Non-LTE Treatment of Fe II in Astrophysical Plasmas

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We describe our implementation of an extremely detailed model atom of singly ionized iron for NLTE computations in static and moving astrophysical plasmas. Our model atom includes 617 levels, 13675 primary permitted transitions and up to 1.2 million secondary transitions. Our approach guarantees that the total iron opacity is included at the correct wavelength with reasonable memory and CPU requirements. We find that the lines saturate the wavelength space, such that special wavelength points inserted along the detailed profile functions may be replaced with a statistical sampling method. We describe the results of various test calculations for novae and supernovae.

I. Introduction

Iron is the most common heavy element in the solar system. With 26 electrons it is quite difficult to treat theoretically as a quantum mechanical system. Because iron is so abundant and because of its low ionization threshold of $\chi_I = 7.87$ eV, the lines of singly ionized iron Fe II are ubiquitous in astrophysical plasmas, from stellar atmospheres to novae, supernovae, and quasars. Since it is so complex, there are many terms and many multiplets in each term. Previous efforts to perform NLTE calculations with Fe II have had to make rather crude approximations, e.g., lumping entire multiplets together in a single "super-level" thereby reducing the model atom to a manageable 30 to 50 levels. The energy spread within a multiplet can correspond to a wavelength spread as large as 200Å, so unless something is done to correct for this, the opacity will not appear at the correct wavelength. For modeling static plasmas such errors are clearly unacceptable and further approximations, e.g., the usage of opacity distribution functions (ODF's) in the radiative transfer equation must be made. In rapidly expanding plasmas, e.g., those found in novae and supernovae, the errors would be uncomfortably large and ODF's cannot be applied. The method we describe in this paper does *not* use any of the aforementioned approximations but includes the lines directly in the radiative transfer equations at the correct wavelength. Therefore, it can be applied to both moving and static media, without either loss of accuracy or further assumptions.

Another problem frequently encountered in classical multi-level NLTE methods is a badly conditioned rate matrix. This will significantly limit the number of individual levels that can be included in the calculation. The method that we introduce in this paper solves these potential problems by solving the statistical equations in a two step procedure, first solving well conditioned linear systems for the departure coefficients and afterwards solving the ionization and dissociation equations using an iterative procedure.

In our effort to produce a multi-purpose multi-level NLTE stellar atmosphere code that is flexible enough to model a wide variety of astrophysical situations, we have developed an Fe II model atom that includes all levels of a multiplet and, therefore, puts the opacity at the correct wavelength.

Figure 1: Grotrian Diagram of the Fe II model atom that we use for the calculations presented here. All 617 level and 13675 b-b transitions which we include in NLTE are shown.

II.   Model Atom

A.   Kurucz Data

We have taken our model atom from the long term projectof R. L. Kurucz,[1] to provide accurate atomic data for modeling stellar atmospheres is an invaluable service to the scientific community. For our current model atom we have kept terms to ^{2}H, which corresponds to the first 29 terms of Fe II . Within these terms we treat all observed levels that have observed b-b "primary" transitions with $\log gf > -3.0$, where g is the statistical weight of the lower level and f is the oscillator strength of the transition. This leads to a model atom with 617 levels and 13675 "primary" transitions which we treat in detailed NLTE; we solve the full rate equations for all these levels including all radiative rates for the primary lines. In addition we treat the opacity and emissivity for the remaining nearly 1.2 million "secondary" transitions in NLTE.

B.   Photo-ionization Rates

Detailed photo-ionization rates for Fe II have yet to be published, although this is one of the goals of the iron project. Thus, we have taken the results of the Hartree Slater central field calculations of Reilman & Manson[2] to scale the ground state photo-ionization rate and have then used a hydrogenic approximation for the energy variation of the cross section. Although these rates are only very rough approximations, they are useful for initial calculations. In the conditions of the test cases we will consider in this paper, the exact values of the b-f cross sections are not important for the opacities themselves (which are dominated by known b-b transitions of Fe II and other species), but they have an influence on the actual b-f rates. This is, of course, unimportant for the computational method which we use and the b-f cross sections can be changed once better data become available.

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C.   Collisional Rates

For collisional rates we have had to make rather rough approximations and, therefore, have approximated bound-free collisional rates using the semi-empirical formula of Drawin.[3] The bound-bound collisional rates are approximated by the semi-empirical formula of Allen,[4] while for permitted transitions we use Von Regemorter's formula.[5] While the collisional rates are important in stellar atmospheres with high electron densities, they are nearly negligible when compared to the radiative rates in the low density envelopes of novae and supernovae which we discuss here as test cases. Small collisional rates constitute a computationally much harder problem so that the tests we present here are good numerical tests of our computational method.

III.   Calculational Method

The large number of transitions of the Fe II ion that have to be included in realistic models of the Fe II NLTE line formation require an efficient method for the numerical solution of the multi-level NLTE radiative transfer problem. As discussed below, the Fe II model atom that we describe includes, more than 13000 individual lines. Classical approaches, e.g., the complete linearization or the Equivalent Two Level Atom methods, would be computationally prohibitive. In addition, we are also interested in modeling moving media, therefore, approaches like Anderson's multi-group scheme[6] or extensions of the opacity distribution function method[7] cannot be applied. Simple approximations like the Sobolev method are very inaccurate in problems in which lines overlap strongly and which have a significant continuum contribution (important for weak lines), as is the case for nova and SN atmospheres.[8]

We, therefore, use the multi-level operator splitting method described by Hauschildt[9] (hereafter Paper II). This method solves the non-grey, spherically symmetric, special relativistic equation of radiative transfer in the comoving (Lagrangian) frame using the operator splitting method described in Hauschildt[10] (hereafter Paper I). It has the advantages that (a) it is numerically highly efficient and accurate, (b) it treats the effects of overlapping lines and continua (including background opacities by lines and continua not treated explicitly in NLTE) self-consistently, (c) gives very stable and smooth convergence even in extreme cases (novae), and (d) it is not restricted to a

certain application but can be applied to a wide variety of astrophysical problems. Details of the method are described in Paper I and II, so we give here only a discussion of the technical improvements necessary to make the NLTE treatment of very large model atoms more efficient.

A.   Full NLTE Treatment: Primary (strong) Lines

Even with highly effective numerical techniques, the treatment of possibly more than one million NLTE lines poses a significant computational problem, in particular in terms of memory usage. In addition, most of these lines are very weak and do not contribute significantly to the radiative rates between their levels. However, they may very well influence the radiation field in overlapping stronger transitions and must therefore be included as background opacity. Therefore, we separate the "primary" lines from the "secondary" lines by defining a threshold in $\log(gf)$, which can be arbitrarily changed. Lines with gf-values larger than the threshold are treated in detail, i.e., they are fully included as transitions in the rate equations. In addition, we include special wavelength points within the profile of the strong lines, whereas the weak lines are treated by opacity sampling (see below). The weaker secondary transitions are included as background NLTE opacity sources but are not explicitly included in the rate equations. Their cumulative indirect effect on the rates is included, as they are considered in the solution of the radiative transfer equation. Note that the distinction between primary and secondary transitions is just a matter of convenience and technical feasibility. It is *not* a restriction of our method or the computer code that we have developed but is easily changed by altering the appropriate input files. As more powerful computers become available, all transitions can be handled as primary lines by simply changing the input files accordingly.

As a typical value, we use a threshold of $\log(gf) = -3$ so that lines with gf-values larger than this threshold are considered as primary lines and all other lines are considered as secondary lines. Note that we do not pose additional thresholds like the energy of the lower level of a line or the statistical weight of the lower level. However, we do include in the selection process only observed lines between observed levels in order to include only lines with well known gf-values. All predicted lines of Kurucz are included as "weak" lines, see below.

Using this procedure to select our model atom, we obtain 13675 primary NLTE lines between the 617 levels included in NLTE. For every line we use 5 to 9 wavelength points within its profile and for all lines the radiative rates and the "approximate rate operators" (see Paper II) are computed and included in the iteration process. We discuss the effect of different treatment of the primary lines, e.g., by opacity sampling, in the results section.

B. Approximate NLTE Treatment: Secondary Lines and LTE Levels

The vast majority of the 1.2 million Fe II lines in the database of Kurucz are either very weak lines or are predicted lines (sometimes between predicted or auto-ionizing levels). Although these weak lines are an important source for the overall opacity and the shape of the resulting "pseudo-continuum" (see below), they are not very important for the rate equations. The transitions between the bound states are dominated by a relatively smaller number of primary transitions, which we include individually in the radiative transfer and rate equation solution.

However, the "haze" of weaker "secondary" lines must be included as background opacity (and hence indirectly in the rate equations). This is also true for the numerous lines of species considered in LTE. Neglecting the line-blanketing would lead to wrong results for the NLTE departure coefficients, see, e.g., Hauschildt & Ensman[11] for a description of this effect found in supernova model atmospheres.

Therefore, we include the opacity of the secondary lines, defined as all available Fe II lines that are not treated individually, as background opacity. Depending on the levels between which a weak transition takes place, we distinguish between

1. lines for which the lower level is an NLTE level but the upper level is an LTE level,

2. lines for which the upper level is an NLTE level but the lower level is an LTE level, and,

3. lines for which both levels are LTE levels.

Here, an 'NLTE level' is a level that is explicitly treated in the NLTE rate equations whereas a 'LTE level' is not considered explicitly in the rate equations. In the first two cases we set the departure coefficient for the LTE level equal to the departure coefficient of the ground state, whereas in the last case we use the same approach as for the lines of LTE species[12–14] except that we use the ground state departure coefficient to include the effects of over or under-ionization. This approximate treatment of the secondary lines does not significantly influence the emergent spectra, as the secondary lines are by definition only relatively weak lines.

IV.   Results

A.   LTE Tests

Before applying our method to simplified test cases, we have performed the usual tests of the computer code and the stability of the model atom. These include tests of the rate and statistical equations with LTE values for either radiative rates alone, for collisional rates alone, and for both LTE radiative rates and collisional rates. We found that deviations of the departure coefficients from their LTE value, $b_i = 1$, is in all cases less than 10^{-6} for a wide range in electron temperatures. These tests were done by simply replacing the results of the monochromatic radiative transfer calculations by their LTE values, but retaining the approximate rate-operators in the calculations. This is very sensitive to small numerical problems in the calculations, e.g., profile normalization errors, which can lead to instabilities in model calculations. Successful tests were very important steps during the development of the large Fe II model atom and its implementation.

B.   The test models

For the test calculations presented below, we have selected a number of simplified nova and supernova model atmospheres. All models were calculated using our general model atmosphere computer code PHOENIX, version 5.3,[8–10,15,16] which implements the numerical method and Fe II model atom as described above. A more detailed description of the input physics and the code itself can be found in the cited references.

Figure 2: Test of the Fe II model atom. We compare 3 different LTE nova test models in the optical (upper panel) and UV spectra ranges. The full curve gives the spectrum calculated using a pure LTE model, i.e., a model in which all lines were taken directly from the LTE line list, including the Fe II lines. The dashed curves (which are practically identical to the full curve) are for a model in which the NLTE lines were computed using the NLTE part of our computer code with all departure coefficients set to unity. This spectrum includes both primary and secondary NLTE lines of Fe II . If we simply omit the secondary Fe II lines, we obtain the spectrum given by the dotted curve.

The nova model atmospheres are calculated using a power law density of the form $\rho(r) \propto r^{-N}$ with $N = 3$. We have used a ballistic velocity law $v(r) \propto r$ with $v_{\mathrm{max}} = 2000\,\mathrm{km\,s^{-1}}$, typically found in nova atmospheres. Nova atmospheres are characterized by a large number of overlapping lines in the ultraviolet and, therefore, the Sobolev approximation *cannot* be used to model either the atmospheres or spectra of novae.[8] Novae are a very important test case because of the complicated structure of their atmospheres, in particular due to their huge electron temperature gradients. We have selected two nova models as test cases: The first has an effective temperature of $T_{\mathrm{eff}} = 15000\,\mathrm{K}$, which is representative of novae around their maximum light in the optical. In this model, the electron temperatures vary from $4500\,\mathrm{K}$ to more than $100000\,\mathrm{K}$. The second nova test model has an effective temperature of $25000\,\mathrm{K}$, it represents a later stage in the nova evolution.

Our supernova test models correspond to the early phase of Type II supernovae with $T_{\mathrm{eff}} = 7000\,\mathrm{K}$ and $9500\,\mathrm{K}$ and maximum expansion velocities of $8000\,\mathrm{km\,s^{-1}}$ and $15000\,\mathrm{km\,s^{-1}}$, respectively. As for the nova models, we have used a power law density, however, for the less extended shells of supernovae we have used a density exponent of $N = 12$ in the hot model and $N = 9$ in the cool model. The hotter model corresponds roughly to conditions much earlier than maximum light, and the cooler model to just before maximum light. We will discuss the NLTE effects of iron on post-maximum SN spectra and Type I supernovae atmospheres and spectra elsewhere. We have used solar compositions for both he nova and supernova models

In order to check the implementation of the model atom and the effect of our distinction between primary and secondary NLTE lines, we have calcu-

Figure 3: Convergence properties of the departure coefficients. The relative corrections $|\Delta b_i|/b_i$ of the ground state departure coefficients are shown as functions of the iteration number. The corrections for a number of different layers in the atmospheres are plotted and the symbols indicate the "standard optical depth" τ_{std} (see text). The results are for a nova model with $T_{\mathrm{eff}} = 15000\,\mathrm{K}$ and a diagonal $[R_{ij}^*]$-operator has been used for all species. The results for the OS/ALI iterations are indicated by the lines connecting the symbols. For comparison we show also the results of the Λ-iterations with unconnected symbols.

lated some LTE test cases. Here, we display the results for the most sensitive test, a nova model atmosphere with $T_{\mathrm{eff}} = 15000\,\mathrm{K}$. In Fig. 2 we compare the spectra computed using a LTE model (all lines were taken from the LTE line list and the NLTE part of the code was switched off) with the spectra obtained replacing the LTE lines of our NLTE species with the lines computed in the NLTE part of the code but setting all departure coefficients to unity. This case is useful in order to understand the effects of the weak Fe II lines on the radiation field and to test the correctness of the code. The two spectra are practically identical, the relative differences are less than 0.1%. Even though in these tests the iron abundance is low, it contributes significantly to the opacity and large differences would significantly effect the output spectra.

In addition, we have calculated a spectrum in which we have artificially neglected the secondary Fe II lines and included only the 13675 primary lines of Fe II (all NLTE lines of the other species as well as the lines of the species treated on LTE were retained) and plotted it in the dotted curve. Even in this case the spectra are nearly identical, we find only minor differences at some UV wavelengths, while in the optical spectral range the differences are localized in a few relatively weak transitions. This demonstrates that our Fe II model atom is large enough and includes enough lines as primary transitions to model the spectrum and the total opacity of Fe II . The secondary lines are a relatively small correction and their influence on the spectrum and the lines formation is, as intended, of secondary importance.

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C. Convergence Properties

To test the convergence properties of the multi-level radiative transfer and rate equations, we have calculated a number of simplified test models. In the nova and supernova test calculations we find that the convergence of the departure coefficients is to a good approximation linear and avoids the stabilization typically found in the Λ-iteration. We show in Fig. 3 the relative corrections to the ground state departure coefficients b_1 of Fe II as functions of the iteration number at a number of optical depth points. We define "standard optical depth scale" τ_{std} as the optical depth in the b-f continuum at $\lambda = 5000$Å. The departure coefficients are defined as the ratio of the NLTE occupation numbers and their LTE values, computed using the NLTE occupation number of the ground state of the next higher ion (see Paper II for details). The two outermost optical depths are outside the line forming region whereas the inner τ points are inside the line forming regions. The last optical depth point plotted is inside the thermalization depth of Fe II . In addition to the operator-splitting—accelerated lambda iteration (OS/ALI) results (indicated by the line connecting the symbols) we have also plotted the results of the simple Λ iteration.

The Fe II converges well and does not show any problematic behavior. The convergence is better at larger optical depths because the exact diagonal $[R_{ij}^*]$-operator (see Paper II) is a better approximation to the discrete rate operator at large optical depths. In smaller and intermediate optical depths the exact tri-diagonal $[R_{ij}^*]$ would lead to much better convergence, but for a model atom as large as the Fe II that we use here, it requires significantly more memory and CPU time per iteration. Thus, in the calculations reported in this paper, we have used only the exact diagonal $[R_{ij}^*]$-operator, which leads to a somewhat lower convergence rate (although the exact tri-diagonal $[R_{ij}^*]$-operator is available in our computer code). At very small optical depths the convergence rates are somewhat better because the radiation field is dominated by the background field emergent from the line forming region and the effects of local radiation fields are much smaller (in effect, this is the transition into the nebular region surrounding a typical nova atmosphere).

We have made the situation more complicated by including a number of other species in the NLTE calculation, as indicated in Fig. 4. These species were not directly coupled to the Fe II model atoms in order to avoid the problematic case of unknown couplings between different species. Fur-

Figure 4: Departure coefficients of the ground state of a number of NLTE species as functions of standard optical depth. The different symbols indicate the different species as shown in the legend of the figure.

thermore, we have only included direct couplings between transitions in the Fe II model atoms in order to save computer time (although the full set of couplings between lines can easily be included in the calculations at the cost of CPU time). As demonstrated in Papers I and II, much better convergence rates are attained if every possible coupling is included in the calculations and if convergence acceleration methods are used. The cases we discuss here should be close to worst case scenarios. That the convergence rates are still acceptable shows the robustness of our numerical method.

D. Departures from LTE

1. Ionization Changes

In Fig. 4 we show the departure coefficients b_1 of the ground states of our NLTE species as functions of τ_{std}. In the nova models, the run of b_1 with optical depth is relatively complicated throughout the line and continuum forming regions. The ground state departure coefficients of Fe II are less than unity in most regions of the atmosphere, indicating an over-ionization of Fe II relative to the LTE situation. At intermediate optical depths ($\tau_{\mathrm{std}} \sim 1 - 100$) the Fe II b_1 are however, larger than unity. This complicated behavior is mirrored by the other NLTE species, in particular by O I. For most species, the change from over to under-ionization occurs over a larger range in optical depth and the "pseudo-nebular" outer region where $b_1 < 1$ is relatively smaller.

Fig. 5 displays the ground state departure coefficient for our hot and cool supernova models. For the hot model the effect of NLTE is over-ionization throughout the line forming region. The cool model displays the complicated behavior seen in the nova models.

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Figure 5:   Departure coefficients of the ground state of Fe II for the hot and cool supernova models as functions of standard optical depth.

2.   NLTE effects of the Fe II lines

Since Fe II is such a complicated atom with so much coupling between levels, it would not be surprising if the main effect of NLTE was over-ionization with the internal population density *ratios* being close to LTE once the over-ionization is taken into account. In Figure 6 we plot the ratio of the departure coefficients to that of the ground state for the levels $z\,^6D^o$, $b\,^4P$, and $z\,^4D^o$ which correspond to the upper level of the $\lambda 2600$ UV1 transition, and the lower and upper levels for the $\lambda 4233$ optical transition, respectively.

If the main effect of NLTE was that the hot radiation field over-ionizes Fe II , then we would expect that the departure coefficient ratio should become constant independent of depth and that the constant would be proportional to $\exp(-\chi/kT_R)$, where T_R is the characteristic temperature of the radiation field, i.e. that a two-fluid approach would be valid. For the cool model, this is never the case and the populations of the levels are far from any kind of thermal equilibrium value. This is not surprising given the *highly* non-Planckian character of the radiation field. Only for the very low optical depths of the hot model does over-ionization appear to be the main effect. In the line formation region, however the behavior is quite complex.

E.   Effects of Fe II NLTE on the emitted spectrum

1.   Nova models

The effects of Fe II NLTE on the spectra emitted by novae are very large. We demonstrate this in Figs. 7 and 8 by comparing the spectra for two nova model atmospheres ($T_{\mathrm{eff}} = 15000\,\mathrm{K}$ and $25000\,\mathrm{K}$) computed assuming LTE population numbers for Fe II and using the full NLTE treatment for the 617 level Fe II model atom. The most obvious effect on the optical spectra, for both effective temperatures, is that Fe II NLTE reduces the emission strength of Hβ (and the higher members of the Balmer series for $T_{\mathrm{eff}} = 25000\,\mathrm{K}$). This is due to a reduced optical depth in the Lyman lines, caused by underpopulation and correspondingly weaker Fe II lines in the wavelength range

Figure 6: The ratio of the departure coefficients to the ground state departure coefficient for our cool (lower panel) and hot (upper panel) test supernova models. The lines correspond to the $z\,^6D^o$ level (the upper level for the $\lambda2600$ UV1 transition), $z\,^4D^o$ level (the upper level for the $\lambda4233$ optical transition), and the $b\,^4P$ level (the lower level for the $\lambda4233$ optical transition).

from 900 to 1250Å. This alters the departure coefficients for hydrogen and thus changes the profiles of the Balmer lines. The effect of Fe II NLTE on the optical Fe II lines seems relatively small, in the 10% range. However, this is important for iron abundance analyses in novae, as this is roughly equivalent to a factor of two change in the Fe abundance.

The situation is very different in the UV spectral range. For the $T_{\text{eff}} = 15000\,\text{K}$ model the NLTE effects of Fe II are not dramatic, in particular the Fe II –Mg II blend at 2800Å is practically unchanged. The feature at 2640Å (actually a gap between strong Fe II lines, see Hauschildt et al.[8]) is slightly "weaker" (i.e., the opacity is enhanced) in the Fe II –NLTE model when compared to the Fe II –LTE model. For the nova atmosphere with $T_{\text{eff}} = 25000\,\text{K}$, however, the changes are significantly larger. The strong Fe II lines which are visible in the Fe II –LTE model at $\lambda \approx 2450$, 2650 (at this effective temperature, this feature is a cluster of Fe II emission lines), and 2770Å are practically wiped out in the Fe II –NLTE model. This is caused by a strong under-population of their levels and a large over-ionization of Fe II in the NLTE case. The Fe II –NLTE model is in much better agreement with actually observed nova spectra (Schwarz et al., in preparation) than the previous LTE model spectra. In addition to this very important effect, the Fe II –NLTE model does not show some of the broad absorption features found in the Fe II –LTE spectrum around 1620Å.

2. Supernova models

Figures 9 and 10 show the effect of Fe II NLTE on the spectra emitted by the supernova models. With the high velocities characteristic of early supernova atmospheres, the individual features are highly blended. None of the effects on the line shapes is as dramatic as in the case of novae. It is interesting, however, that for the cooler models the largest effects are in

Figure 7: The effect of Fe II NLTE on nova spectra. The full curves give the synthetic spectrum of a model atmosphere calculated including the Fe II NLTE effects whereas the dotted curve gives the spectrum calculated using LTE population number for Fe II . All models include, in addition, NLTE effects of H I, He I, O I, Na I, Ne I, Mg II, and Ca II, and line blanketing by other metals. The structures of the atmospheres are identical. The effective temperature of the model atmosphere is $T_{\text{eff}} = 15000\,\text{K}$.

the optical with noticiable changes in Hβ and the Fe II features between 4000 and 5000Å. For the hotter model, the largest changes occur for the Fe II lines in the UV. This is somewhat similar to the nova model. In Type Ia supernovae where iron is a major atmospheric constituent the effects are much larger and we will discuss them in detail in a specialized paper (Nugent et al., in preparation).

These results show that NLTE effects of Fe II are (a) not only important for the formation of the Fe II lines themselves but (b) in addition they can also have an important indirect effect on the formation of the hydrogen lines (at least).

F. Sampling vs special wavelength points

The treatment of primary Fe II transitions by inserting 5 to 7 wavelength points per NLTE line is very accurate, but also very costly in terms of CPU time (its effect on storage is negligible). In order to reduce CPU requirements, we have also implemented an alternate method of treating primary NLTE lines, opacity sampling. The majority of the primary Fe II transitions are in the spectral range from 900Å to 3500Å. In this range, the transitions of Fe II , and other species, lie very close to one another and they overlap strongly. Hence, it is not necessary to insert 5 wavelength points per primary line, if the basic wavelength grid is already fine enough to resolve the line opacity and the radiative rates accurately enough. In the case of moving envelopes of hot stellar objects, such as novae and supernovae, this is actually made simpler by the presence of the $\partial/\partial\lambda$ term in the Lagrangian frame radiative transfer equation. We have tested this method for a smaller Fe II model atom (472 level, 4500 primary transitions) in order to save computer time. The resulting synthetic spectra are practically identical in the test models we

Figure 8:   Same as Fig. 7, but for $T_{\mathrm{eff}} = 25000\,\mathrm{K}$

have calculated, as shown in Fig. 11. We use the sampling procedure only for Fe II lines between 900 and 3500Å, all other primary Fe II NLTE lines, as well as *all* lines of the other NLTE species, are computed using 5 to 7 specially inserted wavelength points per lines. This procedure reduces the number of wavelength points by about a factor of 2 to 3 and reduces the totally CPU time for the model construction also by factors of 2 to 3 (the time required for a model iteration is directly proportional to the number of wavelength points). Another big advantage of the NLTE opacity sampling method is that additional species with many lines in the sampling region (e.g., cobalt, nickel, or titanium), will *not* require additional wavelength points, resulting in a very small increase in computer time as we include more complex NLTE model atoms.

V.   Conclusions

We have implemented a full NLTE treatment for an extremely detailed model atom of Fe II . With 617 levels, 13675 primary and 1.2 million secondary transitions in our Fe II model atom, these calculations are to our knowledge the most detailed NLTE Fe II calculation to date. By making use of the properties of the OS/ALI method developed in Papers I and II, we are able to run our calculations on small workstations (a complete model can be calculated in less than 2 days on an IBM RS/6000 320 workstation, in about 6 hours CPU time on a RS/6000 580, and in about 1.5 hours CPU time on a Cray C90). We have been able to minimize memory and CPU requirements by using a diagonal $[R_{ij}^*]$-operator, but the exact tri-diagonal operator is available for use on larger and faster computers.

Our radiative transfer method is fully relativistic to all orders in v/c and no simplifying assumptions such as the Sobolev approximation have been used. In addition, the detail of our model atom guarantees that the opacity occurs at the correct wavelength so that our calculations are applicable to both static and moving media.

We have been able to further reduce CPU demands by replacing a significant fraction of specially inserted wavelength points for the primary transi-

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Figure 9: The effect of Fe II NLTE on supernova spectra. The dotted curves give the synthetic spectrum of the cool model atmosphere calculated including the Fe II NLTE effects whereas the solid curve gives the spectrum calculated using LTE population number for Fe II . All models include, in addition, NLTE effects of H I, He I, O I, Na I, Ne I, Mg II, and Ca II, and line blanketing by other metals. The structures of the atmospheres are identical.

tions with a statistical sampling technique. This is possible due to the detail of our model atom which ensures that wavelength space is saturated with primary lines. Hence, the inclusion of additional interesting iron peak ions will not substantially increase computational requirements.

We have presented the results of test calculations in novae and supernovae and find that the level populations in the line forming region are quite complex and cannot be simply approximated by a two-fluid approach which assumes that the levels are in internal equilibrium with a hot radiation field and not with the matter. Although this approach would account correctly for the changes in the Fe II ionization equilibrium, it cannot correctly model the line formation of Fe II .

The effects of Fe II NLTE on the spectra of nova and supernova atmospheres are large, in particular for the hotter nova models. With the method we have describe in this paper, it is possible to treat the Fe II NLTE line formation in great detail, and this is required in order to be able to correctly and meaningfully interpret nova and SN spectra. In forthcoming papers we will report the results of detailed analyses of nova and SN spectra using the approach we have described here.

Figure 10:   Same as Fig. 9, but for the hot supernova model.

Figure 11: Effect of sampling on nova spectra.

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